ADVENTURES IN INVARIANT THEORY

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ABSTRACT. We provide an introduction to enumerating and constructing invariants of group representations via character methods. The problem is contextualised via two case studies arising from our recent work: entanglement measures, for characterising the structure of state spaces for composite quantum systems; and Markov invariants, a robust alternative to parameter-estimation intensive methods of statistical inference in molecular phylogenetics.

Keywords: Group character, invariant, plethysm, Schur function, entanglement, SLOCC, tangle, squangle, quartet, general Markov model.

1. BACKGROUND

What can the pursuits of (i) investigating measures of quantum entanglement via multicomponent wavefunctions, on the one hand, and (ii) studying frequency array data in order to infer species evolution in molecular phylogenetics, on the other – both hot topics in their respective fields – possibly have to do with one another? Quite a lot, as it turns out – as becomes clear, once the elegant connections with group representations and tensor analysis are made transparent. The following is an overview of some of the salient background, and a biassed selection of applications of invariant theory in the respective topics. In an appendix we indicate some of the methods and results from character theory needed to establish the required technical theorems which we quote.

Given a group G and a G-module V (a space carrying a linear group action, or representation), there is a standard construct $\mathbb{C}[V^*]$, the space of 'polynomials in the components of the vectors in V'. A natural object is the sub-ring of invariants of G, $I(V) := \mathbb{C}[V^*]^G$. In view of the grading by degree, the coarsest characterisation is the associated Hilbert series, $h(z) = \sum_{0}^{\infty} h_n z^n$ with $h_n = Dim(\mathbb{C}[V^*]^G|_n)$. In well-behaved cases, I(V) has a regular structure (and is finitely generated), and h(z) is a very pleasant rational polynomial. For G semi-simple and compact, Molien's theorem gives a contour integral representation of h(z) via the Haar measure on G. Knowledge of h(z) and of a set of generators of I(V) is generally important for applications. For example if V is the adjoint representation, with G semi-simple, Harish-Chandra's theorem states that I(V) is a polynomial ring, and the algebraically independent generators are nothing but the Casimir operators of the Lie algebra $\mathfrak g$ of G. For an excellent introduction to the theory of representations and invariants of the classical groups see for example [8].

2. APPLICATION – QUANTUM STATES FOR COMPOSITE QUANTUM SYSTEMS

In nonrelativistic quantum mechanics with continuous variable systems, we work with the Schrödinger representation, whose uniqueness is guaranteed by the celebrated Stone-von Neumann theorem. The V's are thus various L^2 spaces and, for multi-particle systems, tensor

products thereof. However, for purely 'spin' systems, the Hilbert spaces can simply be finite-dimensional complex vector spaces $V \cong \mathbb{C}^N$. Our interest here is in composite systems with K subsystems. For $\operatorname{qu} D$ its, then, $N = D^K$. The simplest case occurs for D = 2 and we have K 'qubits', with V the K-fold tensor product $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \mathbb{C}^2$.

This can lead to the oft-described scenario of 'spooky-action-at-a-distance', where, despite remaining in their spatially separated labs, experimenters Alice, Bob, Carol, \cdots , and Karl, through manipulation of their own subsystem, can affect observable outcomes in their colleagues' labs. The properties of each subsystem's quantum state in this case are correlated with those of the other K-1 subsystems. Local unitary transformations, which would be expected in the quantum case, must be extended to the general linear group if Bob $\operatorname{et} \operatorname{al}$ are allowed to communicate the results of their (possibly stochastic) measurements by classical channels, and the symmetry group is taken as $G = \times^K GL(2,\mathbb{C})$. The invariants $\mathbb{C}[V]^G$ are perfectly suited to quantify these non-local quantum effects, and are hence referred to as 'local entanglement invariants'. There is great interest in using these invariants to build complete entanglement measures [28], and the first problem is to characterise and evaluate the invariants in different situations. A famous case in point for tripartite entanglement (K=3) is the use of the Cayley hyperdeterminant, which is called the tangle in the physics literature [5]. See [11] for a recent review of the topic of quantum entanglement.

A less well studied case is that of so-called mixed states, where the state itself is described in a statistical sense (an ensemble of electrons, each of whose members is an electron described by a state vector which is an equal superposition of spin 'up' and spin 'down', is physically very different from an ensemble wherein, in 50% of instances, the electron spin is 'up', and in the other 50%, the electron spin is 'down'). The state is now specified by a density operator (a self-adjoint positive definite linear operator on V of unit trace), and hence transforms in the adjoint representation $\cong V \otimes V^*$. Even just for K=2, that is for *two* qubit mixed states, the structure of the invariant ring is quite rich, for example being considerably more complicated than the *four* qubit pure state case [27]. The Hilbert series [9, 19, 14]

$$h(z) = \frac{1 + z^4 + z^5 + 3z^6 + 2z^7 + 2z^8 + 3z^9 + z^{10} + z^{11} + z^{15}}{(1 - z)(1 - z^2)^3(1 - z^3)^2(1 - z^4)^3(1 - z^6)}$$

enumerates a plethora of primary and secondary invariants, whose precise role in the formulation of suitable entanglement measures is still not completely tied down [9, 19].

3. APPLICATION – PHYLOGENETIC PROBABILITY ARRAYS

What of molecular phylogenetics? The simplest, so-called 'general Markov model' of molecular evolution [2], is given as follows (see also [1]). For a given set of K 'taxonomic units' (species), a probabilistic description of some set of D observed characters is adopted. Models are constructed that describe the frequency of patterns derived from morphological features, or in molecular phylogenetics, from alignments of homologous nucleic acid sequences (nucleotide bases $\{A,C,G,T\}$; D=4), or of homologous proteins (amino acid residues $\{A,R,N,D,C,E,Q,G,H,I,L,K,M,F,P,S,T,W,Y,V\}$; D=20), or a variety of other molecular motifs or repeated units. These models are constructed by assuming molecular sequences evolving from a common ancestor via a Markov process, punctuated by speciation events. The data, corresponding to the observed frequencies, are taken as a sample of the probabilities on the basis that each site in the alignment independently follows an identical random

process. These assumptions are contestible, but are well motivated by considerations of finding a balance between biological realism and statistical tractability. Contained within this model is the description of the evolution of the K extant taxonomic units and their characters. This is a process whereby the K-way probability array, sampled by the pattern frequencies, evolves according to the tensor product of K independent $D \times D$ Markov transition matrices. This scenario is analogous to the set-up of quantum entanglement described above, and algebraically it becomes an instance of the classical invariant theory problem, by extending the semigroup of Markov matrices to the smallest containing matrix group. In the case of continuous-time models, this is no difficulty, as the matrices describing substitution rates between molecular units formally belong to the relevant matrix Lie algebra [26], and the Markov transition matrices are their matrix exponentials — and are hence invertible. From this algebraic perspective, it also makes sense to work over $\mathbb C$ from the outset, and later examine stochastic parameter regions as required for applications.

The said K-fold tensor product module $\mathbb{C}^D \otimes \mathbb{C}^D \otimes \cdots \otimes \mathbb{C}^D$ thus now transforms under $G = GL_1(D) \otimes GL_1(D) \otimes \cdots \otimes GL_1(D)$, where the non-reductive group 1 $GL_1(D,\mathbb{C})$ is the Markov stochastic group of unit row-sum matrices [13, 20] (it is of course a matrix subgroup of GL(D), and is isomorphic to the affine group Aff_{D-1} in one dimension lower). In this case there is no Molien theorem for describing the Hilbert series, and no guarantee of the invariant ring even being finitely generated. However, there is no difficulty in counting invariants degree by degree, and indeed a slightly modified version of the standard results applies (see Appendix). In practical terms this allows us to identify useful invariants for the purposes of phylogenetic inference. In this context we call such objects Markov invariants.

One such quantity, the so-called 'logDet', has in fact been known and in use for over two decades [2, 16, 18]. For the case of two taxa, the determinant function of the 2-fold phylogenetic tensor array (a polynomial of degree D) is certainly a one dimensional representation under the action of $GL(D) \times GL(D)$ itself, in fact transforming as $Det \otimes Det$, and thus necessarily an invariant of the Markov subgroup. Taking the (negative) log, and with the usual matrix relation $-\ln Det = -Tr \ln$, we recover the (negative) sum of the traces of the rate generators, multiplied by the evolved time. Modulo some care with the distribution of characters belonging to the presumed common ancestor of the two taxa, this can be taken as a measure of the total 'edge length' between them, essentially the product of all the individual rates changing characters into one another, multiplied by the time. The 'logDet' can be recorded for all pairs of taxa, using marginalisations of the K-fold probability array, and thus leads to a robust 'distance-based' method for phylogenetic inference, and in fact Buneman's theorem [3] guarantees reconstruction of a tree from a pairwise 'metric' satisfying certain conditions.

Markov invariants beyond the two-fold case are able to be counted and constructed using our technical results, and it is an important matter of principle to identify them. In large data sets, where the pairwise nature of 'logDet' can lead to significant loss of evolutionary information, they may also provide alternative or supplementary information to help with inference. In view of the pevious discussion of quantum entanglement, it turns out that for the case of binary characters (D=2), and three-fold arrays (K=3) or tripartite marginalisations of higher arity arrays, the Cayley hyperdeterminant (degree n=4) is precisely such a candidate [23], and we

¹This group is thus the workhorse of this class of models, playing a role analogous to GL(D), which Weyl in his book famously referred to as 'her all-embracing majesty' amongst the classical groups.

have identified analogous low-degree 'tangles' for D=3 and 4 [24]. For four taxa, and four characters, we have found a symmetrical set of three degree-five Markov invariants dubbed the 'squangles' (stochastic quartet tangles)[22, 25]. A simple least squares analysis of their values allows a direct ranking of one of the three possible unrooted tree topologies for quartets [10]. The squangles provide a low-parameter and powerful way of resolving quartets based on the general Markov model (without any special assumptions about the types of rate matrices in the model) [10], and are useful because many reconstruction methods for large trees build a 'consensus tree' from some kind of ranking of quartet subtrees where robust decisions at the quartet level are absolutely crucial.

It must be noted that Markov invariants are in general distinct from the so-called 'phylogenetic invariants' [4, 15] (see [1] for a presentation in terms of algebraic geometry). Phylogenetic invariants are polynomials that evaluate to zero for a subset of phylogenetic trees regardless of particular model parameters, and in general belong to high-dimensional G-modules.

Our Markov invariants are necessarily quite big objects – they are polynomials of reasonably high degree in a significant number of variables. For example the squangles are degree 5 polynomials in the components of a $4^4=256$ -element array, and given their combinatorial origins, it is perhaps not surprising to find that they each have over 50,000 terms. However, once defined, there is no numerical problem with evaluations – their utility is in their ability to syphon useful information out of the complexity of the data. As such they provide a viable alternative to parameter-estimation intensive phylogenetic methods, where massive likelihood optimisations are required, in order to make decisions about much more tightly specified models.

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APPENDIX A. COUNTING ENTANGLEMENT INVARIANTS: SOME CHARACTER THEOREMS

The mathematical setting for both the study of entanglement measures for composite quantum systems, and of analogous quantities for the setting of phylogenetics, is that there is a model space V which is a K-fold product, $V \cong \mathbb{C}^D \otimes \mathbb{C}^D \otimes \cdots \otimes \mathbb{C}^D$. In the case of quantum mechanics the components of V in some standard basis describe the state; for example in Dirac notation a pure state is a ket $|\Psi\rangle \in V$ of the form $|\Psi\rangle = \sum_{0}^{D-1} \Psi_{i_1 i_2 \cdots i_K} | i_1, i_2, \cdots, i_K \rangle$ in the case of $\operatorname{qu} D$ its (see below for mixed states). In the phylogenetic case we simply have a K-way frequency array $\{P_{i_1 i_2 \cdots i_K}\}$ sampling the probability of a specific pattern, say $i_1 i_2 \cdots i_K$, where each $i_k \in \{A, C, G, T\}$ for nucleotide data, at a particular site in a simultaneous alignment of a given homologous sequence across all K of the species under consideration.

We focus attention on the linear action of the appropriate matrix group $G = G_1 \times G_2 \times \cdots \times G_K$ on V. In the quantum case the local groups G_k would be expected to be $\cong U(D)$, but under conditions where local measurements and correlations of these between parties can occur, the local unitaries are replaced by the complex general linear group $GL(D,\mathbb{C})$. This group is too large for the phylogenetic case, where the pattern frequency array P evolves as $P \to P' := g \cdot P$,

namely

$$P' = M_1 \otimes M_2 \otimes \cdots M_K \cdot P$$

where each M_k belongs to the stochastic Markov group $GL_1(D, \mathbb{C})$ (the group of nonsingular complex unit column-sum $D \times D$ matrices).

We compute the Hilbert series $h(z) = \sum_{0}^{\infty} h_n z^n$ for $\mathbb{C}[V]^G$ degree-by-degree using combinatorial methods based on classical character theory for GL(D), and adapted slightly for the stochastic case $GL_1(D)$. All evaluations are carried out using the group representation package © Schur [30].

In terms of class parameters (eigenvalues) x_1, x_2, \cdots, x_D for a nonsingular matrix $M \in GL(D)$, the defining representation, the character is simply $Tr(M) = x_1 + x_2 + \cdots + x_D$; the contragredient has character $Tr(M^{T-1}) = x_1^{-1} + x_2^{-1} + \cdots + x_D^{-1}$. Irreducible rational and polynomial characters of GL(D) are given by the celebrated Schur functions [29, 17] denoted $s_{\lambda}(x)$, where $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_D)$, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$, is an integer partition; $\ell(\lambda)$, the length of the partition, is the index of the last nonzero entry (thus $\ell(\lambda) = D$ if $\lambda_D > 0$). For brevity we write simply $\{\lambda\}$ where the class parameters are understood. Thus the space V as a representation of G is endowed with the K-fold product character $\chi = \{1\} \cdot \{1\} \cdot \cdots \cdot \{1\}$ in the quantum mechanical pure state and stochastic cases, and $\chi = \{1\} \cdot \{1\} \cdot \cdots \cdot \{1\} \cdot \{1\}$ in the quantum mechanical mixed state case, where $\{1\}$ is the defining representation, and $\{\overline{1}\}$ the contragredient. The space of polynomials of degree n in Ψ or P, $\mathbb{C}[V]_n$, is a natural object of interest and by a standard result is isomorphic to the n-fold symmetrised tensor product $V \vee V \vee \cdots \vee V$, a specific case of a Schur functor: $\mathbb{S}_{\{n\}}(V)$. Its character is determined by the corresponding Schur function plethysm, $\chi \underline{\otimes} \{n\}$, and the task at hand is to enumerate the one-dimensional representations occurring therein.

Before giving the relevant results it is necessary to note two further rules for combining Schur functions. The *outer* Schur function product, is simply the pointwise product of Schur functions, arising from the character of a tensor product of two representations. Of importance here is the *inner* Schur function product defined via the Frobenius mapping between Schur functions and irreducible characters of the symmetric group. We provide here only the definitions sufficient to state the required counting theorems in technical detail. For a more comprehensive, Hopfalgebraic setting for symmetric functions and characters of classical (and some non-classical groups) see [6, 7].

Concretely, we introduce structure constants for inner products in the Schur function basis as follows:

$$\{\lambda\}*\{\mu\} = \sum_{\nu} g^{\nu}_{\lambda,\mu}\{\nu\}.$$

For partitions λ , μ of equal weight, $|\lambda| = |\mu| = n$, say, this expresses the reduction of a tensor product of two representations of the symmetric group \mathfrak{S}_n labelled by partitions λ , μ . By associativity, we can extend the definition of the structure constants to K-fold inner products,

$$\{\tau_1\} * \{\tau_2\} * \cdots * \{\tau_K\} = \sum_{\nu} g^{\nu}_{\tau_1, \tau_2, \cdots, \tau_K} \{\nu\}$$

Theorem: counting entanglement invariants

(a) Quantum pure states:

Let $D \vdash n$, n = rD, and let τ be the partition (r^D) (that is, with Ferrers diagram a

rectangular array of r columns of length D). Then

$$h_n = g^{(n)}_{ au, au,\dots, au}$$
 (K -fold inner product).

If $D \not\vdash n$, then $h_n = 0$.

(b) Quantum mixed states: We have

$$h_n = \sum_{|\tau| = n, \ell(\tau) \le D^2} \left(\sum_{|\sigma| = n, \ell(\sigma) \le D} (g_{\sigma, \sigma}^{\tau})^2 \right)$$

(c) Phylogenetic K-way pattern frequencies, general Markov model:

Let n = rD + s, $s \ge 0$. Then

$$h_n = g_{\tau_1, \tau_2, \cdots, \tau_K}^{(n)}$$
 (K-fold inner product),

for each τ_k of the form $(r+s, r^{(D-1)})$.

(c) Phylogenetic K-way pattern frequencies, doubly stochastic model:

Let
$$n = r(D-1) + s + t$$
, $0 \le t \le r$, $s \ge 0$. Then

$$h_n = g_{\tau_1, \tau_2, \dots, \tau_K}^{(n)}$$
 (K-fold inner product),

for each τ_k of the form $(r+s, r^{(D-2)}, t)$.

As pointed out in the main text, the enumeration and identification of entanglement invariants, in the case of quantum systems, and Markov invariants, in the phylogenetic context, is of practical importance in characterising general properties of the systems under study – in the quantum case, because they are by definition impervious to local operations, and in the phylogenetic case because they tend to be independent of the specific Markov change model and because they can give information about the underlying tree. In the case of the squangles, we find $g^{(5)}_{\ \tau\tau\tau\tau}=4$, where τ is the partition $(2,1^3)$ which is of course of dimension 4 in GL(4) but is indecomposable, and contains a one-dimensional representation of $GL_1(4)$. Of the four candidates, one is redundant because of algebraic dependence on lower degree invariants. Recourse to the appropiate quartet tree isotropy group [25] shows indeed that there are only two nonzero algebraically independent degree five invariants; we parametrize these in terms of three quantities Q_1 , Q_2 , Q_3 such that $Q_1+Q_2+Q_3=0$.

There are many more gems to be examined in hunting down Markov invariants for different models and subgroups [12], with potential practical and theoretical interest. As one further instance of as-yet unexplored terrain, for K=3 we have evidence [21, 22] at degree 8 for stochastic tangle ('stangle') invariants with mixed weight, since it turns out that

$$g_{(51^3),(2^4),(2^4)}^{(8)} = 1 \quad (\equiv g_{(2^4),(51^3),(2^4)}^{(8)} \equiv g_{(2^4),(2^4),(51^3)}^{(8)}) \, .$$

Thus there are three mixed weight stangle candidates, which would differ in the information they reveal about each leg of their ancestral star tree.

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